ABSTRACT OF THE DISCLOSURE

Descriptors of cohesive interactions in the solid state are calculated from a computational model of a solid state, i.e. from a small cluster of copies of the molecule of interest assembled using a molecular mechanics method. A model for predicting solubility is built using the cohesive interaction descriptors along with other descriptors useful for this purpose. Predicted solubility is computed for the compound of interest by computing the same descriptors and applying the solubility model. Explicit modeling of solid state allows to more accurately characterize cohesive interactions in solids, hence, more accurately predict solubility.